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Science Day 2005 Poster Abstracts: Theory and Computation

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Theory and Simulations UCRL-PROC-211170

Dynamic Data-Driven Event Reconstruction for Atmospheric Releases

Branko Kosovic

Atmospheric releases of hazardous materials have a rapid, high-consequence impact on large populations. For emergency response, sensor network design, and forensic needs, we are developing an event-reconstruction capability for use at the National Atmospheric Release Advisory Center. Our approach couples data and predictive models with Bayesian inference and stochastic sampling to provide backward analyses to determine unknown source characteristics, optimal forward predictions for consequence assessment, and dynamic reduction in uncertainty as additional data become available.

We use stochastic sampling methods to solve source inversion problems and compute source term parameters, taking into consideration measurement errors and forward model errors. Stochastic sampling methods are suitable even for the problems characterized by non-Gaussian distribution of source-term parameters. In this poster, we demonstrate our Markov Chain Monte Carlo (MCMC) event-reconstruction capability using data from the Prairie Grass and Copenhagen tracer field experiments. By using data from a subset of sensors and the operational Lagrangian particle dispersion code LOFI, the source location and source release rate can be identified. We have also developed and implemented a Stochastic Monte Carlo (SMC) capability to assimilate data dynamically as they become available.

How Does Atmospheric Turbulence Change in an Urban Environment?

Julie Lundquist

Due to their large populations, urban areas are particularly vulnerable to high-consequence accidental or intentional atmospheric releases of hazardous materials, and because of their complexity, urban environments present challenges for simulating atmospheric transport and dispersion.

To quantify the urban effect on atmospheric dispersion and to provide a dataset for the testing and validation of urban dispersion models, the Joint URBAN 2003 (JU2003) field experiment was funded by the Departments of Energy, Homeland Security, and Defense. LLNL, in collaboration with several other national laboratories and universities, mounted hundreds of meteorological and tracer instruments in and around the Oklahoma City urban core during July 2003. These instruments documented the evolving atmosphere and the effect of the Oklahoma City urban area on the state of the atmosphere. By releasing SF6, a passive tracer gas, in the city center, JU2003 groups (including a large LLNL contingent) explored the unique characteristics of dispersion in the urban area. Ongoing efforts in the Atmospheric Science Division are using these data for testing, validating, and improving the numerical models used in the National Atmospheric Release Advisory Center. This poster focuses on some unique aspects of urban meteorology revealed by the JU2003 experiment, particularly by the LLNL downwind profile.

Hindered Transport Phenomena in Complex Media

David Clague

The study of hindered transport phenomena involves the behavior of particles (e.g., colloids, macromolecules, and carrier particles) in complex media. Both convective processes—entrainment of particulate species with the suspending fluid—and diffusive processes govern particle rates of transport. In pure fluid, the entrained particles move with the velocity of the fluid and experience Brownian motion if they are at the colloidal scale. However, in a complex medium, like a physiological membrane, the suspended species experience hydrodynamic and colloidal interactions with the "fixed" surrounding medium, in this case the colloidal membrane, which contribute to hydrodynamic drag.

Starting in 1905, Einstein published a series of papers on Brownian motion and diffusion. From this body of work came the celebrated Stokes-Einstein equation for a Brownian sphere diffusing in a pure fluid. The equation derives from the balance of chemical potential and viscous resistance. However, in complex media, only the Stokes drag, not the viscous resistance, can be described. The drag must include hydrodynamic contributions from the fixed surrounding medium. Self-diffusive processes in complex media are said to be described by the generalized Einstein equation, which incorporates all of the hydrodynamic interactions experienced by diffusing particles. We use the generalized Einstein equation to describe diffusive processes in microfluidic devices, diffusion in polymers, and filtration processes relevant to Laboratory missions. Synergistically, the models and capabilities developed for Laboratory missions are directly applicable to describing and understanding diffusive processes at the physiological and cellular levels.

On the Movement of Small Particles in Liquids: Heat and Compression

Eric Schwegler

Recent advances in both experimental techniques and sophisticated theoretical methods have resulted in the discovery of fascinating new properties of materials under extreme conditions. In many instances, measurements alone are insufficient for a complete understanding of the emerging new phenomena. In such cases, ab initio methods have proven to be a useful complement for resolving ambiguities. First principles methods are also especially valuable for the prediction of properties where measurements do not yet exist. Our investigations on fluids are aimed at predicting and characerizing structural, electronic, and dynamical properties of materials under high temperature and pressure conditions by using a combination of different theoretical methods, including density functional theory, quantum Monte Carlo methods and quantum molecular dynamics.

Generalized Brownian Motion in Coarse-Grained Molecular Dynamics

Robb Rudd

Can Einstein's understanding of the random motion of pollen grains help us to resolve why cracks propagate at the wrong speed in computer simulations? It can, if we follow Einstein and focus on the unseen. In the computer simulation of materials, it is often desirable to direct computational power to the regions of the system where it is needed most. In finite element analysis, this motivation led to the development of adaptive mesh refinement; in atomistic simulation, the problem is more challenging, but the relatively recent development of concurrent multiscale simulation permits atomistic resolution of part of the system, coupled to a coarse-grained representation of other regions of the system. The coarse-grained model can be a conventional finite element model, and the resulting savings in computational expense permits the simulation of much larger systems. The invention of coarse-grained molecular dynamics (CGMD) made it possible to derive a generalized finite element formalism from the underlying atomistic dynamics directly for the first time. CGMD naturally recovers the atomistic force laws as the mesh is refined to the atomic scale. One result of this rigorous theory of concurrent multiscale coupling is that the coarse-grained modes are not deterministic; they experience random and dissipative forces due to the effective heat bath of the short wavelength modes that have been integrated out. Remarkably, this generalized Brownian motion resolves a long-standing issue with pathological energy flow when atomistic simulations are embedded in coarse-grained surroundings (including vacuum), best known from spurious wave reflections in fracture simulations that affect the crack propagation velocity. Thus, the action of the unseen degrees of freedom, just as in the motion of Brown's pollen grains, leads to unexpected and mystifying phenomena.

Quantum Simulation of High-*Z* Metals at Extreme Conditions

Randy Hood

First-principles quantum simulations based on density-functional theory (DFT) have become a key area of research within the materials science, chemistry and condensed-matter physics communities. We have pioneered the development and use of these methods for high-*Z* metals with ground-breaking simulations of d- and f-electron materials on ASCI White, the Los Alamos National Laboratory's Q machine, and Thunder. We are now adapting our quantum molecular-dynamics (QMD) simulation code to meet the challenges of the revolutionary BlueGene/L (BG/L) machine, where new application horizons await, including materials aging and high-pressure melting. To harness the power of such large-scale computational platforms, it is critical to employ local methods to solve the DFT equations in order to minimize interprocessor communications. In the context of plane-wave-based QMD methods, substantial progress has already been made in this regard by localizing the required fast Fourier transforms (FFTs). Other real-space approaches such as the finite-element method are also being developed, and the successful adaptation of these to BG/L will provide tremendous new opportunities to study the properties of high-*Z* metals at extreme

conditions. The poster presents available QMD simulation results from White, Q, Thunder and BG/L.

For more information, see http://www-phys.llnl.gov/Research/Metals_Alloys/index.html

Atomic-Scale Simulation of Rapid Resolidification in a Molten Metal on BlueGene/L

Fred Streitz

One-hundred years ago this month Albert Einstein published one of the seminal papers of the 20th century in which he described how Brownian motion, the apparently random motion of particles suspended in a liquid, arises from the thermal motion of atoms or molecules in a liquid. This paper is credited with ushering in a broader belief in the existence of atom and molecules, an issue that had been debated since antiquity. Although the acceptance of atoms is now taken for granted, we still seek to understand the apparently random motion of atoms in a liquid. Our investigative tool of choice is LLNL's BlueGene/L (BG/L), the largest computer in the world. With large-scale molecular dynamics, we use BG/L to model the motion of hundreds of thousands of atoms in a liquid metal undergoing rapid compression to understand the process of solidification at extremes of pressure and temperature. Using advance quantum-based potentials to describe interatomic interactions and bond orientational order parameters to characterize the local structure, we demonstrate how the nucleation of a solid phase from the liquid is actually a gradual process stemming from countless random fluctuations in the liquid. A video sequence of the simulation demonstrates the stochastic nature of the event, one of the first successful scientific applications on BG/L.

First-Principles, Linear-Scaling Electronic Structure Calculations

Jean-Luc Fattebert

Using modern computational methods, one can access molecular dimensions and even more complex details at the microscopic level, such as the nature of molecule–molecule interactions. We have devised and are implementing a new approach for accurate first-principles electronic structure calculations, whose complexity is proportional to the size of the system. This is a significant improvement over state-of-the-art methods, which generally scale as the cube of the number of atoms being simulated. The new method is based on localized electronic orbitals and real-space discretization, along with adaptive mesh refinement and multigrid methodologies to speed up computation. The superior scaling opens the door to solving problems that were previously considered intractable.

Concerning a Point of View on the Emission and Transformation of Light in Nanoparticles*

Andrew Williamson

Semiconductor nanoparticles are an exciting new class of materials with unique abilities to transform the properties of light. By controlling the size, shape, and composition of nanoparticles, their optical absorption and emission can be tuned from the infrared through to the ultraviolet, while maintaining high quantum efficiencies. These nanoparticles are already used in a range of nanotechnology applications, including biological imaging, telecommunications and solar cells. Here we present the results of quantum mechanical simulations of the optical properties of silicon, germanium, carbon, and cadmium selenide nanoparticles. These simulations have been used both to interpret existing optical characterization experiments and to predict novel structures of nanoparticles with enhanced optical properties.

*Einstein's 1905 photoelectric effect paper is entitled "Concerning an heuristic point of view toward the emission and transformation of light."

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